Superconductivity in a magnetically ordered background

A. Amici, P. Thalmeier, and P. Fulde
Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany

Borocarbide compounds with the formula RNi_2B_2C show interesting superconducting and magnetic properties and the coexistence of the two phenomena. BCS theory is extended to systems with underlying commensurate magnetic order. In the case of helical phases the technique may be extended to any **Q**-vector and there exists a well defined limit for incommensurate values. The way magnetic order influences superconductivity depends crucially on the details of both the magnetic structure and the electron bands, but some qualitative criteria may be given. As an example we give a brief analysis of the compound $HoNi_2B_2C$.

The borocarbides are a class of compounds with formula RNi_2B_2C (R = Y, La, or a rare earth). They attract attention because of their interesting superconducting and magnetic properties and their mutual interaction. Compounds with Y, Lu, Tm, Er, Ho and Dy have phonon mediated superconductivity at relatively high temperatures [1]. On the magnetic side Gd, Tb, Dy, Ho, Er and Tm show long-range magnetic order with a variety of different structures [2]. Crystalline electric field effects determine the easy direction of the spins in the localised f-states of the rare earth ions, while the RKKY interaction among them determines the ordering **Q** vector. Commensurate and incommensurate magnetic structures coexist with superconductivity. The case of $HoNi_2B_2C$ has been the most spectacular, where a c-axis incommensurate helix, an a-axis incommensurate phase and a c-axis antiferromagnet appear in the same temperature region in which the superconducting upper critical field shows a pronounced depression [3,4].

For the description of superconductivity in the coexistence region we use an extended BCS theory. The Hamiltonian of band electrons interacting with a given exchange field is:

$$H_M = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}}\, c^+_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \sum_{\mathbf{k}\mathbf{q}\sigma\sigma'} \mathbf{h}_{\mathbf{q}} \cdot \boldsymbol{\sigma}^{\sigma\sigma'}\, c^+_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma'}, \quad (1)$$

where $\mathbf{h}_{\mathbf{q}}$ is the Fourier transform of the internal effective magnetic field ($\mathbf{h}_{\mathbf{q}} = \mu_B\, g\, I(\mathbf{q})\, \mathbf{S}(\mathbf{q})$) and $\boldsymbol{\sigma}^{\sigma\sigma'}$ is a vector with the Pauli matrices as the components. Conventional notation is used for the other symbols [5]. This has to be added to the usual phonon Hamiltonian:

$$H_{SC} = \sum_{\mathbf{q}} \omega_{\mathbf{q}}\, a^+_{\mathbf{q}} a_{\mathbf{q}} + \sum_{\mathbf{k}'\mathbf{k}\sigma} g_{\mathbf{k}'\mathbf{k}}\, c^+_{\mathbf{k}'\sigma} c_{\mathbf{k}\sigma} \left(a_{\mathbf{k}'-\mathbf{k}} + a^+_{\mathbf{k}-\mathbf{k}'}\right) \quad (2)$$

For a given exchange field $\mathbf{h}_{\mathbf{q}}$ commensurate with the lattice the eigenstates problem for H_M is reduced to solving a $n \times n$ matrix, where n is the number of rare earth atoms in the magnetic unit cell. Using the extended unit cell representation, the total Hamiltonian of the system is given by:

$$H = \sum_{\mathbf{k}\nu} \tilde{\epsilon}_{\mathbf{k}\nu}\, \tilde{c}^+_{\mathbf{k}\nu} \tilde{c}_{\mathbf{k}\nu} + \sum_{\mathbf{q}} \omega_{\mathbf{q}}\, a^+_{\mathbf{q}} a_{\mathbf{q}} + \\ + \sum_{\mathbf{k}'\mathbf{k}\nu'\nu} \tilde{g}^{\nu'\nu}_{\mathbf{k}'\mathbf{k}}\, \tilde{c}^+_{\mathbf{k}'\nu'} \tilde{c}_{\mathbf{k}\nu} \left(a_{\mathbf{k}'-\mathbf{k}} + a^+_{\mathbf{k}-\mathbf{k}'}\right) \quad (3)$$

The main differences with respect to the non-magnetic case are:
(1) the magnetic eigenstates are labeled by the index ν that does not refer to a definite spin state. Furthermore energy spin degeneracy is in general lifted and magnetic Cooper pairs formed with these states will not be in spin singlet state
(2) the band structure acquires gaps at magnetic Bragg planes and possibly at other characteristic surfaces. Whenever the Fermi surface intersects one of those planes or surfaces it is force to become orthogonal to it. However, apart from pathological situations, the properties of the electrons are affected only to order $\frac{h}{\epsilon_F}$
(3) the scattering amplitude between magnetic states $\tilde{g}^{\nu'\nu}_{\mathbf{k}'\mathbf{k}}$ acquires further **k** dependence linked to the underlying exchange field. Typical magnetic energy bands are shown in the figure .

Introducing the gap function matrix:

$$\Delta^{\nu'\nu} = \langle \tilde{c}_{\mathbf{k}\nu'} \tilde{c}_{-\mathbf{k}\nu} \rangle \quad (4)$$

we are able to construct the mean-field theory of superconductivity in a way quite close to the standard one. Some qualitative remarks are now possible: in magnetic states with a net magnetisation (i.e. ferromagnets) $\nu = \sigma$, spin degeneracy is lifted and coexistence is possible only for very small values of the magnetisation. On the other hand, if the net magnetisation is zero and the magnetic structure is collinear to a given vector $\hat{\mathbf{n}}$ ($\mathbf{S}(\mathbf{x}) = S(\mathbf{x}) \cdot \hat{\mathbf{n}}$), the spin along that direction is conserved. In these cases (i.e., antiferromagnets [6] and longitudinally modulated phases) the magnetic theory reduces to the usual one but with modified band structures and interaction with phonons.

At a qualitative level it may be noticed that:
(1) if magnetic order does not destroy large pieces of the Fermi surface, as in the case of nesting, electronic properties are only slightly modified and the opening of the magnetic gap does not imply strong suppression of superconductivity
(2) time-reversal symmetry of the system is not a necessary condition for the existence of superconducting pairs, nor is time-reversal plus a translation symmetry [6]

Now we consider the case of helical magnetic order. For a helix with wave vector $\mathbf{Q}$ and amplitude h, the magnetic eigenstates may be computed analytically through a Bogoliubov transformation:

$$\tilde{\epsilon}_{\mathbf{k}\pm} = \frac{\epsilon_{\mathbf{k}\pm\mathbf{Q}} + \epsilon_{\mathbf{k}}}{2} + \frac{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}\pm\mathbf{Q}}}{2}\sqrt{1 + \frac{4h^2}{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}\pm\mathbf{Q}})^2}}$$

and the Bogoliubov coefficients are:

$$u(\mathbf{k}) = \sqrt{\frac{1}{2}\left[1 + \sqrt{\frac{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{Q}})^2}{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{Q}})^2 + 4h^2}}\right]}$$

$$v^2(\mathbf{k}) = 1 - u^2(\mathbf{k})$$

Cooper pairs formed with these electronic states are in a mixed state of singlet and triplet. Using the Einstein approximation for the phonon dispersion law (ω_0) and the structureless electron-phonon interaction ($g_{\mathbf{k}'\mathbf{k}} = g$) in the weak coupling limit it is possible to obtain the standard BCS equation for the gap function with a modified definition of the interaction parameter (see Ref. [7] for more details):

$$\tilde{\lambda} = \frac{2g^2}{\omega_0} \int\limits_{MFS} dS \, \frac{\left(u^2(\mathbf{k}) - v^2(\mathbf{k})\right)^2}{|\nabla_{\mathbf{k}}\tilde{\epsilon}_{\mathbf{k}}|}$$

In order to give a quantitative estimate for the new effective electron-phonon coupling constant we assume cylindrical symmetry around the z-axis for the energy bands and linearise them at the magnetic gap. In this way band effects enter through the two components of the Fermi velocity ($\hbar\mathbf{v}_F = \nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}$): the one orthogonal ($v_\perp$) and the one parallel ($v_\parallel$) to the z-axis. The difference in the interaction parameter is given by:

$$\Delta\lambda = \tilde{\lambda} - \lambda = -\frac{g^2}{\pi\,\hbar^2\omega_0}\,\frac{k_r}{v_\perp v_\parallel}\,h$$

where $k_r \sim k_F$ is the radius of the intersection between the Fermi surface and the magnetic Bragg plane. The relative reduction of the superconducting parameter is then:

$$\frac{\Delta\lambda}{\lambda} \sim -\frac{(\hbar v_F k_r)\,h}{(\hbar v_\perp k_F)\,(\hbar v_\parallel k_F)} \qquad (5)$$

Eq. (5) has the following qualitative features:
(1)assuming $v_\perp$ and $v_\parallel$ of order v_F the variation of the interaction parameter is proportional to $\frac{h}{\epsilon_f}$ and λ is reduced only by a few percent
(2) however RKKY interaction maxima are usually connected to pieces of the Fermi surface orthogonal to the $\mathbf{Q}$ vector close to the Bragg planes. If the $\mathbf{Q}$ vector of the magnetic order is determined by the RKKY interaction (as it happens generally for incommensurate structures), then $v_\perp \ll v_F$ and the suppression of superconductivity may be large. These qualitative features may give an interpretation of the behaviour of superconductivity in $HoNi_2B_2C$. From anisotropic magnetisation measurement a broad maximum in the RKKY function is inferred close to $q = (0, 0, \pi)$ [8]. This maximum is related to both the magnetic c-axis incommensurate helix and to the c-axis antiferromagnet. Because of its flatness it is probably due to the overall structure of the electronic bands and not to sharp nesting features, thus $v_\perp \sim v_F$. On the other hand the a-axis modulation appears to be related to nesting features of the Fermi surface (both experimentally and through band calculations [9]). We therefore suggest that the a-axis modulation has a stronger destructive character for superconductivity than the c-axis modulation [10].

We conclude that an extended BCS theory may be constructed in the general case of commensurate magnetic structures. In the special case of helical magnetic order the extended theory is also valid in the incommensurate limit. A possible qualitative explanation for the anomalies in the superconductivity of $HoNi_2B_2C$ has been suggested.

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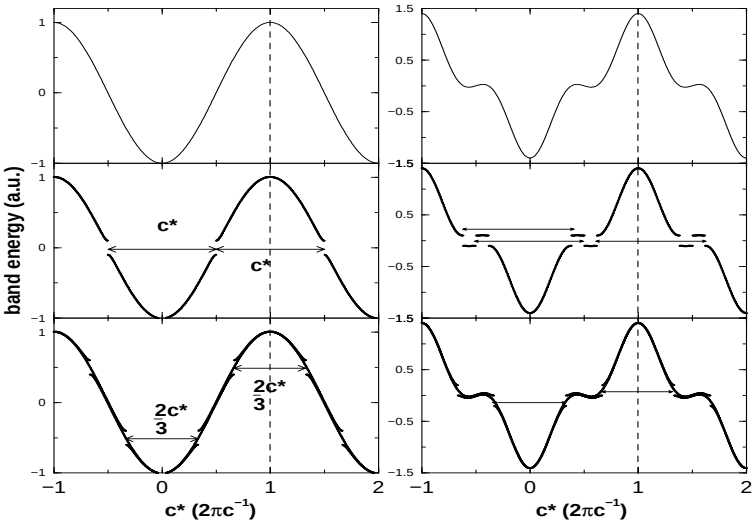

FIG. 1. Effect of the magnetic order on two model band structures. The magnetic vector used are $q = \pi$ in the middle row, corresponding to antiferromagnetic order, and $q = \frac{2\pi}{3}$ in the lower row, corresponding to structure with periodicity of three unit cells. Note that magnetic gaps here correspond to $\frac{h}{\epsilon_F} \sim 0.1$ in order to emphasise them, physical values for the gaps are 10 to 100 times smaller.